ACNS 2008 Tutorial

A hands-on look at quasielastic neutron scattering for the investigation of mobility in soft condensed matter.

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Maximum Number of Participants: 20

Quasielastic neutron scattering (QENS) is a valuable technique for the investigation of dynamics in soft condensed matter systems: polymers, molecular liquids, complex fluids, and biological systems. This technique couples spatial sensitivity at the Å scale with observation of relaxation processes in the time window ranging from few picoseconds to hundreds of nanoseconds. Thus, QENS enables investigation of dynamics at a molecular level. Moreover, the high scattering cross section of hydrogen atoms allows for highlighting specific parts of the sample using selective deuteration.

QENS remains under-utilized among soft matter scientists in the American neutron scattering community. The goal of this tutorial is thus to provide an introduction to QENS, emphasizing its application to the study of soft condensed matter. The course will present the principles of the three main QENS techniques: Time-of-Flight (ToF), Backscattering, and Neutron Spin-Echo (NSE). Given the overlapping time and spatial scales of Molecular Dynamics (MD) simulations with QENS experiments, and the utility of simulation to guide experimental interpretation, the final session of the tutorial will introduce the MD technique. The tutorial will be based on both

presentations and interactive data analysis sessions, which emphasize how QENS can address current scientific problems.

The course is primarily aimed at students and post-doctoral researchers who have a basic knowledge of neutron scattering techniques and are new to quasielastic neutron scattering. Lecture notes from the tutorial will be made available to the participants.

Schedule:

9.00-10.00 Introduction to Quasielastic Neutron Scattering (QENS)

(J.R.D. Copley)

This introductory presentation will present background information needed to understand the remainder of the tutorial. A general knowledge of neutron scattering will be assumed. The following concepts will be introduced:

- Relaxation phenomena.
- Quasielastic scattering.
- Coherent and Incoherent Scattering.
- Time and Space scales investigated by QENS.
- Energy resolution (time scale).
- Comparison of the different types of QENS spectrometers (ToF, Backscattering, and Spin-Echo) with reference to the different space-time scales involved.

10.00-12.00 QENS in the energy domain: Time of Flight and Backscattering instruments.

(A. Sokolov)

The time will be divided in two sections: a presentation and an interactive session with the data analysis of previously collected data.

The presentation should address the following topics:

- The time-space scales investigated by the spectrometers.
- The basic technical principles of the instruments.
- Examples of relevant scientific problems addressed with the use of QENS.

- How to prepare a successful QENS experiment.
- Hands-on exercise.

12.00-13.30 Lunch Break

13.30.15.30 QENS in the time domain: Neutron Spin-Echo

(A. Faraone)

The time will be divided in two sections: a presentation and an interactive session with the data analysis of previously collected data.

The presentation should address the following topics:

- The time-space scales investigated by the spectrometer.
- The basic technical principles of the instrument.
- Examples of relevant scientific problems addressed with the use of NSE.
- How to prepare a successful NSE experiment.
- Hands-on exercise.

15.30-15.45 Coffee Break

15.45-17.45 Molecular Dynamics (MD) simulations and QENS

(Grant Smith, Coray Colina)

This session will provide two examples of the use of molecular dynamics simulation with QENS data.

-The first speaker will give a basic overview of the MD technique [what it does, ensemble, thermostats & barostats, what a force field is], followed by a research example.
-The second speaker will give information about how to get started on MD [system sizes that are feasible, how to choose a force field, codes to use, etc.], followed by a research example.